The classical limit of the time dependent Hartree-Fock equation. II. The Wick symbol of the solution.

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The first aim of this paper is to derive under minimal hypotheses Ehrenfest's theorem concerning the time evolution of the Wick symbol for a quantum observable (i.e, its average taken on coherent states). This theorem (see [CTDL]) says that the Wick symbol follows the classical mechanics equations as the semiclassical parameter h goes to 0. This result shall be precisely stated in section 1 and proved in section 6 for observables that are not pseudo-differential operators and consequently in the case where this theorem cannot be deduced from Egorov's theorem. One may see [R2], [CF], [CR1], [CR2], [S], [U1], [U2] for references concerning coherent states and some of their applications and Ammari-Nier [AN1][AN2] in the case of the infinite dimension.

Following our preceding work [AKN], the second purpose here is to study the time evolution of the Wick symbol of a trace class operator solution to the time dependent Hartree Fock equation (TDHF). The work in [AKN] is devoted to the Weyl symbol of such of an operator $\rho_h(t)$ under the hypothesis that the initial operator $\rho_h(0)$ is a pseudo-differential trace class operator belonging to the the class of operators studied by C. Rondeaux [R] (actually, the class of operators in [R] is independent on h and the parameter h is inserted here in order to consider semi-classical operators). Under weaker hypotheses than those assumed in [AKN] we shall study here the Wick symbol of such a solution, instead of its Weyl symbol. A solution to (TDHF) is a trace class operator and its Wick symbol is a function belonging to $L^1(\mathbb{R}^{2n})$. We shall prove that the time evolution of the Wick symbol for a solution to the (TDHF) equation "tends to the time evolution associated to the Vlasov equation" as the limit h goes to 0. This limit shall be understood in the $L^1(\mathbb{R}^{2n})$ sense. The precise statement of this result is written in section 2 (see theorem 2.1) and its proof is given in section 7.

One of the tools used in order to established both of these two results is the approximation of a bounded operator in $L^2(\mathbb{R}^n)$, (resp. of a trace class operator), verifying rather weak hypotheses, by pseudo-differential operators lying in the class of Calderon-Vaillancourt [CV] (resp. in the class of C. Rondeaux [R]). This process is similar to a convolution where translations are now replaced by an action in the Heisenberg group. The details are found in section 5.

In order to motivate the introduction of the Wick symbol it is given in section 3 an explicit example of a trace class operator having a Weyl symbol which is not in $L^1(\mathbb{R}^{2n})$. On the contrary, the Wick symbol of a trace class operator is always in $L^1(\mathbb{R}^{2n})$ (this point is proved by C. Rondeaux [R]) together with all of its derivatives (this fact is derived in section 4). Moreover, an asymptotic expansion of the Wick symbol for the product of two operators when one of them is a semi-classical pseudo-differential operator and when the other one is any trace class operator is written in section 8. The bound for the remaining term of this asymptotic expansion is effectuated in the $L^1(\mathbb{R}^{2n})$ norm. Note that an analysis for the commutator of an operator defined by the Weyl calculus with another operator defined with the anti-Wick formalism is found in R. Schubert [S] (theorem 4.1.12). The results in section 8 below can be formally seen as the dual in some sense of those in R. Schubert. One may also see lemma 2.4.6 of N.Lerner [L1]. In section 9 it is obtained an equation being approximatively satisfied by the Wick symbol of a solution to (TDHF) with an arbitrary small error term (see [DLERS] for the idea of such an equation). Finally in section 10, it is observed that the

convergence's result established in corollary 2.2 is not uniform on $\mathbb{R}$ even if the two potentials are entirely vanishing.

1. Statement of the result : the case of bounded operators and Ehrenfest's theorem.

In this section the time evolution of the system is associated to the following Hamiltonian (which depend on $h > 0$)

$$\widehat{H}_h = -h^2 \Delta + V \tag{1.1}$$

where V is a C^∞ real-valued function on $\mathbb{R}^n$ which is bounded together with all of its derivatives. We also denote by $\widehat{H}_h$ the unique self-adjoint extension of this operator. Let $(A_h)_{h>0}$ be a family of bounded self-adjoint operators in $L^2(\mathbb{R}^n)$. The operator $A_h(t)$ corresponding to the evolution of the operator A at the time t is

$$A_h(t) = e^{i\frac{t}{h}\widehat{H}_h} A_h e^{-i\frac{t}{h}\widehat{H}_h}. \tag{1.2}$$

According to the standard statements of Ehrenfest's theorem (see [CTDL]) the average of $A_h(t)$ taken on coherent states is supposed to approximatively follow the classical mechanics's laws as h tends to 0 .

The coherent state centered at the point $X = (x, \xi)$ in $\mathbb{R}^{2n}$ is the following function, depending on $h > 0$

$$\Psi_{X,h}(u) = (\pi h)^{-n/4} e^{-\frac{|u-x|^2}{2h}} e^{\frac{i}{h}u.\xi - \frac{i}{2h}x.\xi} \qquad X = (x, \xi) \in \mathbb{R}^{2n}. \tag{1.3}$$

The average taken on Ψ_{Xh} of a bounded operator A in $\mathcal{H} = L^2(\mathbb{R}^n)$ is

$$\sigma_h^{wick}(A)(X) =< A\Psi_{Xh}, \Psi_{Xh} > . \tag{1.4}$$

The function $\sigma_h^{wick}(A)$ is called the Wick symbol of A. When A is a bounded operator we shall notice (see proposition 4.1) that the function $\sigma_h^{wick}(A)$ is C^∞ on $\mathbb{R}^{2n}$ and we shall give precise estimations on its derivatives in terms of the parameter h and of the norm of A. Let us now specify in which sense does this function follows the classical mechanics equations under the limit h tends to 0.

Let $\varphi_t(x, \xi) = (q_t(x, \xi), p_t(x, \xi))$ denotes the Hamiltonian flow of the function $H(x, \xi) = |\xi|^2 + V(x)$ starting at (x, ξ), i.e., the solution to,

$$q_t'(x, \xi) = 2q(t, x, \xi) \qquad p_t'(x, \xi) = -\nabla V(q(t, x, \xi)) \tag{1.5}$$

such that $q_0(x, \xi) = x$, $p_0(x, \xi) = \xi$. One can say that a function $f(x, \xi, t)$ "follows the classical mechanics laws" when $f(X, t) = f(\varphi_t(X), 0)$ for all $X \in \mathbb{R}^{2n}$ and all $t \in \mathbb{R}$.

If the initial data A_h is not assumed to be a semiclassical pseudo-differential operator (see D. Robert [R1]), then the function $\sigma_h^{wick}(A_h(t))$ may not have a limit as $h \to 0$. Nevertheless, we shall precisely state in which sense this function "follows the classical mechanics's equations under the limit h tends to 0". Our goal is to prove under rather weak hypotheses and for all time $t \in \mathbb{R}$ that,

$$\lim_{h\to 0} \left| \sigma_h^{wick}(A_h(t))(X) - \sigma_h^{wick}(A_h(0))(\varphi_t(X)) \right| = 0 \tag{1.6}$$

In particular, this is not $\sigma_h^{wick}(A_h(t))(X)$ that has a limit when $h \to 0$ but the difference between this function and another one which follows the classical mechanics laws and takes the same value as $\sigma_h^{wick}(A_h(t))(X)$ at time 0.

Let us now precisely state the hypotheses implying the validity of the limit (1.6). We shall denote by $W^{mp}(\mathbb{R}^{2n})$ the space of functions in $L^p(\mathbb{R}^{2n})$ having all of its derivatives up to order m in $L^p(\mathbb{R}^{2n})$ ($1 \leq p \leq +\infty$, $0 \leq m \leq +\infty$).

First, let us recall how the Egorov theorem is classically applied the case of operators A_h which are semiclassical pseudodifferential operators. In this case, A_h is associated, through the Weyl calculus, to a function F_h in $W^{\infty\infty}(\mathbb{R}^{2n})$, which is bounded in $W^{\infty\infty}(\mathbb{R}^{2n})$ independently of $h \in (0,1]$. Namely, for all $f \in \mathcal{H}$,

$$(A_h f)(x) = (2\pi h)^{-n} \int_{\mathbb{R}^{2n}} F_h(\frac{x+y}{2}, \xi) e^{\frac{i}{h}(x-y).\xi} f(y) dy d\xi \tag{1.7}$$

According to Calderon-Vaillancourt [CV], A_h is bounded in $\mathcal{H}$. We agree to express (1.7) under the two following expressions

$$A_h = Op_h^{weyl}(F_h) \qquad\qquad F_h = \sigma_h^{weyl}(A_h) \tag{1.8}$$

(The Weyl symbol of an arbitrary bounded operator being a priori in $\mathcal{H}$ is a tempered distribution on $\mathbb{R}^{2n}$.) If F_h is either independent of h or admitting an asymptotic expansion in the powers of h as h tends to 0, Egorov's theorem shows that:

$$\lim_{h \to 0} \left(\sigma_h^{weyl}(A_h(t))(X) - \sigma_h^{weyl}(A_h(0))(\varphi_t(X)) \right) = 0 \tag{1.9}$$

In that case, the limit (1.6) then follows. Indeed,

$$\sigma_h^{wick}(A_h(t)) = e^{\frac{h}{4}\Delta} \sigma_h^{weyl}(A_h(t)) \tag{1.10}$$

(Even if this result is standard, we shall nevertheless give a proof in proposition 4.4.) Besides, Egorov's theorem also shows that, if A_h is written as in (1.7) with F_h in $W^{\infty\infty}(\mathbb{R}^{2n})$ and uniformly bounded in $h \in (0,1]$ then $\sigma_h^{weyl}(A(t))$ is also a function in $W^{\infty\infty}(\mathbb{R}^{2n})$, bounded uniformly on $h \in (0,1]$. As a consequence,

$$\lim_{h \to 0} \left(\sigma_h^{wick}(A_h(t))(X) - \sigma_h^{weyl}(A_h(t))(X) \right) = 0 \tag{1.11}$$

for all $t \in \mathbb{R}$. In this case, the limit (1.6) then follows from (1.9) and (1.11).

The assumption $A = Op_h^{weyl}(F)$ with F in $W^{\infty\infty}(\mathbb{R}^{2n})$ is rather strong and may be expressed in terms of commutators in a standard way. Let $P_j(h)$ and $Q_j(h)$ be the momemtum and the position operators,

$$P_j(h) = \frac{h}{i} \frac{\partial}{\partial x_j} \qquad\qquad Q_j(h) = x_j \tag{1.12}$$

According to Beals characterization result [B], the fact that A_h may be written as $A_h = Op_h^{weyl}(F)$ with F in $W^{\infty\infty}(\mathbb{R}^{2n})$ is equivalent to the fact that the commutators $(ad\ P(h))^\alpha (ad\ Q(h))^\beta A$ are bounded (for all multi-indexes α, β). Saying that F (which may depend on h) stays bounded in $W^{\infty\infty}(\mathbb{R}^{2n})$ is equivalent to the fact,

$$h^{-(|\alpha|+|\beta|)} \|(ad\ P(h))^\alpha (ad\ Q(h))^\beta A\|_{\mathcal{L}(\mathcal{H})} \leq M_{\alpha\beta}$$

with $M_{\alpha\beta}$ independent on h.

We are first concerned with the proof of the limit (1.6), which may possibly be viewed as a form of Ehrenfest's theorem, but under much weaker hypotheses than in the case where A_h is a semiclassical operator. Namely, only single commutators (instead of iterated commutators) of the operator A_h with the operators $P_j(h)$ and

$Q_j(h)$ defined in (1.12) are assumed to be bounded operators. Our estimates shall involve the following expression,

$$I_h^\infty(A) = \frac{1}{h}\sum_{j=1}^{n} \|[P_j(h), A]\|_{\mathcal{L}(\mathcal{H})} + \|[Q_j(h), A]\|_{\mathcal{L}(\mathcal{H})} \tag{1.13}$$

The theorem below provides the inequality on which rely the proof of Ehrenfest's theorem with weakened hypotheses.

Theorem 1.1 *For all operators A in $\mathcal{L}(\mathcal{H})$ such that the commutators $[P_j(h), A]$ and $[Q_j(h), A]$ are bounded operators in $\mathcal{H}$ ($1 \leq j \leq n$), the operator $A_h(t)$ defined in (1.2) and the Hamiltonian flow φ_t defined in (1.5) satisfy*

$$\left\| \sigma_h^{wick}(A_h(t)) - \left(\sigma_h^{wick}(A)\right) \circ \varphi_t \right\|_{L^\infty(\mathbb{R}^{2n})} \leq C(t)\sqrt{h} I_h^\infty(A) \tag{1.14}$$

where $t \mapsto C(t)$ is a function defined on $\mathbb{R}$, bounded over any compact set, depending only on n and on V and where $I_h^\infty(A)$ is defined in (1.13).

In order that (1.6) can be viewed as Ehrenfest's theorem it suffices to replace A by a family of operators A_h such that the right hand-side of (1.13) tends to 0 as h goes to 0. This assumption is satisfied when $A_h = Op_h^{weyl}(F_h)$ with F_h in $W^{\infty\infty}(\mathbb{R}^{2n})$ and uniformly bounded in $h \in (0, 1]$.

2. Statement of the result: the case of trace class operators and the time dependent Hartree Fock equation.

Before introducing the time dependent Hartree Fock equation (TDHF) let us first specify the space to which the solution belongs. We shall denote by $\mathcal{L}^1(\mathcal{H})$ the space of all trace class operators on $\mathcal{H} = L^2(\mathbb{R}^n)$. We shall denote by $\mathcal{D}$ the subspace of operators A in $\mathcal{L}^1(\mathcal{H})$ such that the commutator $[\Delta, A]$ is also in $\mathcal{L}^1(\mathcal{H})$ where Δ is the Laplacian.

We consider two real-valued functions V and W in $W^{\infty\infty}(\mathbb{R}^n)$. For all $h > 0$ we shall say that a function $t \to \rho_h(t)$ being C^1 from $\mathbb{R}$ into $\mathcal{L}^1(\mathcal{H})$ is a classical solution to the time dependent Hartree Fock (according to the terminology of Bove da Prato Fano [BdF1,BdF2]) when this mapping is also continuous on $\mathbb{R}$ into $\mathcal{D}$ and if,

$$ih\frac{\partial}{\partial t}\rho_h(t) = -h^2[\Delta, \rho_h(t)] + [V_q(\rho_h(t)), \rho_h(t)] \tag{2.1}$$

where $V_q(\rho_h(t))$ denotes the multiplication operator by the function:

$$V_q(x, \rho_h(t)) = V(x) + Tr(W_x \rho_h(t)) \tag{2.2}$$

where W_x is the multiplication operator by the function $y \to W(x - y)$.

We consider a family $(\rho_h(t))_{h>0}$ of classical solutions to (TDHF). We suppose that the operator $\rho_h(0)$ is trace class, self-adjoint ≥ 0 with a trace equal to 1. We set:

$$u_h(X, t) = (2\pi h)^{-n}\sigma_h^{wick}(\rho_h(t))(X) \tag{2.3}$$

As we shall see in section 4 this function lies in $W^{\infty 1}(\mathbb{R}^{2n})$, it is ≥ 0 and

$$\int_{\mathbb{R}^{2n}} u_h(X,t)dX = 1 \tag{2.4}$$

We denote by $v_h(X,t)$ the solution to the Vlasov equation,

$$\frac{\partial v_h}{\partial t} + 2\sum_{j=1}^{n} \xi_j \frac{\partial v_h}{\partial x_j} - \sum_{j=1}^{n} \frac{\partial V_{cl}(x, v_h(.,t))}{\partial x_j} \frac{\partial v_h}{\partial \xi_j} = 0 \tag{2.5}$$

such that

$$v_h(X,0) = u_h(X,0) \tag{2.6}$$

We have set,

$$V_{cl}(x, v_h(.,t)) = V(x) + \int_{\mathbb{R}^{2n}} W(x-y) v_h(y,\eta,t) dy d\eta \tag{2.7}$$

The function $v_h(.,t)$ is itself in $L^1(\mathbb{R}^{2n})$, it is ≥ 0 and its integral equals to 1.

The counterpart of Ehrenfest's theorem for a family of solutions to (TDHF) consists into saying that the function $u_h(.,t)$ defined in (2.3) satisfies Vlasov equation "under the limit h tends to 0". This point of view may specified in different ways. In this section our aim is to compare as in theorem 1.1 the functions $u_h(.,t)$ and $v_h(.,t)$ and to show that, under suitable assumptions on $\rho_h(0)$, their difference in norm tends to 0. Since we are concerned with trace class operators it makes sense that the norm involved in the estimation of the difference $u_h(.,t) - v_h(.,t)$ is the $L^1(\mathbb{R}^{2n})$ norm. A first answer to this issue is given in our preceding article (preprint) [AKN] where we assume that the operator $\rho_h(0)$ is a pseudo-differential operator belonging to a class of operators introduced by C. Rondeaux [R] (the only modification here being the insertion of the parameter h). The article [AKN] also gives an asymptotic expansion at any order of $u_h(.,t) - v_h(.,t)$. We consider here this problem with a weaker hypothesis than the one in [AKN]. We are only assuming that all the commutators $[P_j(h), \rho_h(0)]$ and $[Q_j(h), \rho_h(0)]$ are trace class operators. All these estimates shall use the expression,

$$I_h^{tr}(\rho_h(0)) = \frac{1}{h}\sum_{j=1}^{n} \|[P_j(h), \rho_h(0)]\|_{\mathcal{L}^1(\mathcal{H})} + \|[Q_j(h), \rho_h(0)]\|_{\mathcal{L}^1(\mathcal{H})} \tag{2.8}$$

Theorem 2.1. *Let $(\rho_h(t))_{h>0}$ be a family of classical solutions to (TDHF) with real-valued potentials V and W in $W^{\infty\infty}(\mathbb{R}^{2n})$. We suppose that the operator $\rho_h(0)$ is trace class, self-adjoint ≥ 0, with a trace equal to 1. We assume that all the commutators $[P_j(h), \rho_h(0)]$ and $[Q_j(h), \rho_h(0)]$ are trace class operators. Then, there exists a function $t \mapsto C(t)$, bounded on any compact set of $\mathbb{R}$ such that, for all $h \in (0,1]$ and for all $t \in \mathbb{R}$,*

$$\|u_h(.,t) - v_h(.,t)\|_{L^1(\mathbb{R}^{2n})} \leq C(t)\sqrt{h} I_h^{tr}(\rho_h(0)) e^{C(t) I_h^{tr}(\rho_h(0))} \tag{2.9}$$

Corollary 2.2. *Under the assumptions of theorem 2.1, if $I_h^{tr}(\rho_h(0))$ remains bounded when h tends to 0, then we have,*

$$\lim_{h\to 0} \|u_h(.,t) - v_h(.,t)\|_{L^1(\mathbb{R}^{2n})} = 0 \tag{2.10}$$

for all $t \in \mathbb{R}$.

If $\rho_h(0)$ is a pseudo-differential operator written as $\rho_h(0) = (2\pi h)^n Op_h^{weyl}(F_h)$ with F_h in $W^{\infty 1}(\mathbb{R}^{2n})$ and uniformly bounded in h then the assumption in corollary 2.2 is always satisfied according to the analogous result of the Beals's characterization given in [R] (see [AKN] for dependence on the parameter h).

Theorem 2.1 shall be proved in section 7. An other way to give an insight into Ehrenfest's theorem consists into proving that the function $u_h(X,t)$ satisfies an equation that formally shrink to the Vlasov equation when h tends to 0. It is this point of view that we shall develop in section 9.

3. A counter-example.

By making explicit an idea of C. Rondeaux [R] we shall give an example of a trace class operator having a Weyl symbol not being in $L^1(\mathbb{R}^{2n})$. Let us mention before some properties for the Weyl symbol of a trace class operator that lead us to the choice of the counter-example.

Proposition 3.1. *If A is trace class, then its Weyl symbol is a continuous function on $\mathbb{R}^{2n}$ going to 0 at infinity and also belonging in $L^2(\mathbb{R}^{2n})$. If this function is also ≥ 0 then it is necessarily in $L^1(\mathbb{R}^{2n})$.*

Proof. If A is trace class then it is also Hilbert-Schmidt and it is well-known that its Weyl symbol belongs to $L^2(\mathbb{R}^{2n})$ (cf D. Robert [R1]). This symbol is bounded since when A is trace class we have,

$$\sigma_h^{weyl}(A)(X) = 2^n Tr(A \circ \Sigma_{Xh}) \qquad X \in \mathbb{R}^{2n} \tag{3.1}$$

The fact that it is continuous and that it is going to 0 at infinity is easily verified using (3.1) for an operator written as $u \to A(u) =< u, \varphi > \psi$, where φ and ψ are in $\mathcal{S}(\mathbb{R}^n)$. One then concludes this point by density, first for any finite rank A, then for any trace class operator since the set of finite rank operators is dense in $\mathcal{L}^1(\mathcal{H})$. For all functions F in $W^{\infty 1}(\mathbb{R}^{2n})$ and G in $W^{\infty\infty}(\mathbb{R}^{2n})$ it is well-known (cf D. Robert [R1]) that,

$$Tr(Op_h^{weyl}(F) \circ Op_h^{weyl}(G)) = (2\pi h)^{-n} \int_{\mathbb{R}^{2n}} F(X)\, G(X)\, dX \tag{3.2}$$

Let A be a trace class operator and G be a C^∞ function on $\mathbb{R}^{2n}$ with compact support. From theorem 5.2 there exists a sequence of functions (F_j) in $W^{\infty 1}(\mathbb{R}^{2n})$ such that the sequence of operators $Op_h^{weyl}(F_j)$ converges to A in $\mathcal{L}^1(\mathcal{H})$, implying from (3.1) that F_j converges uniformly to $\sigma_h^{weyl}(A)$. It is then deduced that,

$$Tr(A \circ Op_h^{weyl}(G)) = (2\pi h)^{-n} \int_{\mathbb{R}^{2n}} \sigma_h^{weyl}(A)(X)\, G(X)\, dX \tag{3.3}$$

We replace G by an increasing sequence G_N of C^∞ functions on $\mathbb{R}^{2n}$ with compact support and converging pointwise to 1 when N goes to $+\infty$, the functions $|\partial_x^\alpha \partial_\xi^\beta G_N|$ being all uniformly bounded on N. When $\sigma_h^{weyl}(A) \geq 0$ we deduce from (3.3) that,

$$0 \leq (2\pi h)^{-n} \int_{\mathbb{R}^{2n}} \sigma_h^{weyl}(A)(X)\, G_N(X)\, dX \leq \|A\|_{\mathcal{L}^1(\mathcal{H})}\, \|Op_h^{weyl}(G_N)\|_{\mathcal{L}(\mathcal{H})}$$

According to Calderon-Vaillancourt the right hand-side remains bounded as N tends $+\infty$. If the function $\sigma_h^{weyl}(A)$ is ≥ 0 then it is therefore in $L^1(\mathbb{R}^{2n})$.

□

Proposition 3.1 and the results of C. Rondeaux [R] suggest the construction of an example of a trace class operator having a Weyl symbol not being in $L^1(\mathbb{R}^{2n})$. We may assume that $h = 1$. Let α be a real number such that $\frac{n}{2} < \alpha \leq n$. We define the operator P by:

$$P = Op_1^{weyl}(p) \qquad p(x,\xi) = \frac{e^{2ix.\xi}}{(1+|x|^2+|\xi|^2)^\alpha} \qquad (x,\xi) \in \mathbb{R}^{2n}. \tag{3.4}$$

The function p is not in $L^1(\mathbb{R}^{2n})$. For all $\lambda > 0$ we define an operator A_λ by

$$A_\lambda = Op_1^{weyl}(a_\lambda) \qquad\qquad a_\lambda(x,\xi) = e^{2ix\xi - \lambda(|x|^2+|\xi|^2)}.$$

We have:

$$P = \frac{1}{\Gamma(\alpha)} \int_0^\infty e^{-\lambda}\lambda^{\alpha-1} A_\lambda d\lambda \tag{3.5}$$

provided that we verify the convergence. From definition (1.7) the integral kernel of A_λ is the function K_λ defined by:

$$K_\lambda(x,y) = (2\pi)^{-n} \int_{\mathbb{R}^n} e^{i(x-y)\cdot\xi} a_\lambda\left(\frac{x+y}{2}, \xi\right) d\xi.$$

An explicit computation shows that:

$$K_\lambda(x,y) = (2\pi\lambda)^{-n/2}\ e^{-(a(\lambda)|x|^2 + b(\lambda)|y|^2 + 2c(\lambda)x.y)} \qquad a(\lambda) = \frac{\lambda}{4} + \frac{1}{\lambda} \qquad b(\lambda) = c(\lambda) = \frac{\lambda}{4}.$$

We can express the operator A_λ as a product,

$$A_\lambda = (2\pi\lambda b(\lambda))^{-n/2}\ T_{a(\lambda)} \circ B_\lambda \circ T^{-1}_{b(\lambda)} \circ S \tag{3.6}$$

where for all $a > 0$, $(T_a f)(x) = f(x\sqrt{a})$, $Sf(x) = f(-x)$ and:

$$(B_\lambda f)(x) = \int_{\mathbb{R}^n} e^{-(|x|^2+|y|^2)+2\mu(\lambda)x.y} f(y) dy \qquad \mu(\lambda) = \frac{c(\lambda)}{\sqrt{a(\lambda)b(\lambda)}}. \tag{3.7}$$

The operator B_λ is self-adjoint ≥ 0 (since $0 < \mu(\lambda) < 1$ and $B(\lambda)$ may be identified, up to a multiplicative constant, to the exponential of an harmonic oscillator). We then see:

$$\|B_\lambda\|_{\mathcal{L}^1(\mathcal{H})} = \mathrm{Tr}(B_\lambda) = \int_{\mathbb{R}^n} e^{-2(1-\mu(\lambda))|x|^2} dx = \left(\frac{\pi}{2(1-\mu(\lambda))}\right)^{n/2}.$$

From (3.6) we have,

$$\|A_\lambda\|_{\mathcal{L}^1(\mathcal{H})} \leq (2\pi\lambda b(\lambda))^{-n/2}\ \|T_{a(\lambda)}\|_{\mathcal{L}(\mathcal{H})}\ \|B_\lambda\|_{\mathcal{L}^1(\mathcal{H})}\ \|T^{-1}_{b(\lambda)}\|_{\mathcal{L}(\mathcal{H})}.$$

The right hand-side is polynomially increasing as $\lambda \to +\infty$ and it is $\mathcal{O}(\lambda^{-n/2})$ when λ tends to 0. With the choice of $\alpha > \frac{n}{2}$, the integral (3.5) converges in norm in $\mathcal{L}^1(\mathcal{H})$ and it properly defines a trace class operator P, the Weyl symbol of which is the function p defined in (3.4), and is not belonging to $L^1(\mathbb{R}^{2n})$.

For trace class operators, it is natural to give a variant of Ehrenfest's theorem where the limit is understood in the $L^1(\mathbb{R}^{2n})$ sense. The above counter-example shows that the Weyl symbol is not suitable for this purpose without any supplementary hypothesis. However, proposition 4.2 below shows that the Wick symbol of a trace class operator is C^∞ from $\mathbb{R}^{2n}$ into $L^1(\mathbb{R}^{2n})$ together with all of its derivatives.

4. Differentiability of the Wick symbol.

Proposition 4.1. *Let A be a bounded operator in $\mathcal{H}$. Then the Wick symbol of A, namely, the function $\sigma_h^{wick}(A)$ defined on $\mathbb{R}^{2n}$ by (1.4), is a C^∞ function on $\mathbb{R}^{2n}$, bounded together with all of its derivatives. For each multi-index α there exists C_α such that:*

$$\|\nabla^\alpha \sigma_h^{wick}(A)\|_{L^\infty(\mathbb{R}^{2n})} \leq C_\alpha h^{-|\alpha|/2}\ \|A\|_{\mathcal{L}(\mathcal{H})}. \tag{4.1}$$

Proof. We shall use the following function,

$$S_h(A)(X,Y) = \frac{< A\Psi_{Xh}, \Psi_{Yh} >}{< \Psi_{Xh}, \Psi_{Yh} >}, \tag{4.2}$$

defined on $\mathbb{R}^{2n} \times \mathbb{R}^{2n}$, where the functions Ψ_{Xh} are given in (1.3). Direct computations shows that:

$$< \Psi_{Xh}, \Psi_{Yh} >= e^{-\frac{1}{4h}|X-Y|^2 + \frac{i}{2h}\mathrm{Im}(X.\overline{Y})}. \tag{4.3}$$

In particular,

$$| < \Psi_{Xh}, \Psi_{Yh} > | = e^{-\frac{1}{4h}|X-Y|^2} \qquad \|\Psi_{Xh}\| = 1. \tag{4.4}$$

Consequently:

$$\Big| S_h(A)(X,Y) \Big| = e^{\frac{1}{4h}|X-Y|^2} | < A\Psi_{Xh}, \Psi_{Yh} > | \leq e^{\frac{1}{4h}|X-Y|^2} \, \|A\|_{\mathcal{L}(\mathcal{H})}. \tag{4.5}$$

An important property verified by coherent states is that:

$$< f, g >= (2\pi h)^{-n} \int_{\mathbb{R}^{2n}} < f, \Psi_{Xh} > < \Psi_{Xh}, g > \; dX \tag{4.6}$$

for all f and g in $\mathcal{H}$. Applying this equality, we see that:

$$\sigma_h^{wick}(A)(X) = S_h(A)(X,X) = (2\pi h)^{-2n} \int_{\mathbb{R}^{4n}} \mathcal{B}_h(X,U,V,X) S_h(A)(U,V) dUdV \tag{4.7}$$

where for all (X,U,V,Y) we have set:

$$\mathcal{B}_h(X,U,V,Y) = \frac{< \Psi_{Xh}, \Psi_{Uh} >< \Psi_{Uh}, \Psi_{Vh} >< \Psi_{Vh}, \Psi_{Yh} >}{< \Psi_{Xh}, \Psi_{Yh} >}. \tag{4.8}$$

From (4.3) we have:

$$\mathcal{B}_h(X,U,V,X) = e^{-\frac{1}{2h}(X-V)(\overline{X}-\overline{U}) - \frac{1}{2h}|U-V|^2}. \tag{4.9}$$

We verify that:

$$h^{m/2} |\nabla_X^{\alpha} \mathcal{B}_h(X,U,V,X)| \leq C_m K_m(X,U,V,h) e^{-\frac{1}{4h}|U-V|^2}$$

where

$$K_m(X,U,V,h) = \left(1 + \frac{|X-U| + |X-V|}{\sqrt{h}} \right)^m \; e^{-\frac{1}{4h}(|X-U|^2 + |V-X|^2)}.$$

Consequently:

$$h^{m/2} \Big| \nabla_X^m \sigma_h^{wick}(A)(X) \Big| \leq C_m (2\pi h)^{-2n} \int_{\mathbb{R}^{4n}} | < A\Psi_{Uh}, \Psi_{Vh} > | K_m(X,U,V,h) \; dUdV. \tag{4.10}$$

By bounding from above $| < A\Psi_{Uh}, \Psi_{Vh} > |$ by the norm of A we then obtain (4.1).

Proposition 4.2. *If A is in $\mathcal{L}^1(\mathcal{H})$, then its Wick symbol $\sigma_h(A)$ belongs to $W^{\infty 1}(\mathbb{R}^{2n})$. For each multi-index α there exists $C_\alpha > 0$ such that,*

$$(2\pi h)^{-n} \|\nabla^m \sigma_h^{wick}(A)\|_{L^1(\mathbb{R}^{2n})} \leq C_m h^{-\frac{m}{2}} \|A\|_{\mathcal{L}^1(\mathcal{H})}. \tag{4.11}$$

Inequality (4.11) is proved when $m = 0$ by C. Rondeaux [R].

Proof. Similarly to proposition 4.1, we have inequality (4.10). Integrating with respect to X we obtain:

$$h^{m/2}(2\pi h)^{-n}\|\nabla^m \sigma_h^{wick}(A)\|_{L^1(\mathbb{R}^{2n})} \leq C_m(2\pi h)^{-2n}\int_{\mathbb{R}^{4n}} |< A\Psi_{Uh}, \Psi_{Vh} > G_m\left(\frac{U-V}{\sqrt{h}}\right) \quad dUdV$$

$$G_m(U) = (1+|U|)^m e^{-\frac{|U|^2}{8}}.$$

Since the function G_m is in $L^1(\mathbb{R}^{2n})$, proposition 3.2 is a consequence of the following lemma.

Lemma 4.3. *Let A be a trace class operator and G be a function in $L^1(\mathbb{R}^{2n})$. Then we have:*

$$(2\pi h)^{-2n}\int_{\mathbb{R}^{4n}} \left| < A\Psi_{Xh}, \Psi_{Yh} > G\left(\frac{X-Y}{\sqrt{h}}\right)\right| dXdY \leq (2\pi)^{-n}\|G\|_{L^1(\mathbb{R}^{2n})}\|A\|_{\mathcal{L}^1(\mathcal{H})}. \tag{4.12}$$

Proof. We can write $A = B_1B_2$ where B_1 and B_2 are two Hilbert-Schmidt operators. Using the fundamental indentity (4.6) verified by the coherent states we see that, for all X and Y in $\mathbb{R}^{2n}$,

$$< A\Psi_{Xh}, \Psi_{Yh} > = < B_2\Psi_{Xh}, B_1^\star\Psi_{Yh} > = (2\pi h)^{-n}\int_{\mathbb{R}^{2n}} u_{Zh}(X)\ v_{Zh}(Y)\ dZ$$

where we have set $u_{Zh}(X) = < B_2\Psi_{Xh}, \Psi_{Zh} >$ and $v_{Zh}(X) = < \Psi_{Zh}, B_1^\star\Psi_{Xh} >$. Let I_h be the left hand-side of (4.12). From Schur's lemma:

$$I_h \leq (2\pi h)^{-3n}h^n\|G\|_{L^1(\mathbb{R}^{2n})}\int_{\mathbb{R}^{2n}} \|u_{Zh}\|_{L^2(\mathbb{R}^{2n})}\ \|v_{Zh}\|_{L^2(\mathbb{R}^{2n})}dZ.$$

From (4.6), we have $\|u_{Zh}\|_{L^2(\mathbb{R}^{2n})} = (2\pi h)^{n/2}\|B_2^\star\Psi_{Zh}\|$ and $\|v_{Zh}\|_{L^2(\mathbb{R}^{2n})} = (2\pi h)^{n/2}\|B_1\Psi_{Zh}\|$. Consequently,

$$I_h \leq (2\pi h)^{-2n}h^n\|G\|_{L^1(\mathbb{R}^{2n})}\int_{\mathbb{R}^{2n}} \|B_1\Psi_{Zh}\|\ \|B_2^\star\Psi_{Zh}\|\ dZ.$$

From the basic indentity (4.6) for coherent states,

$$(2\pi h)^{-n}\int_{\mathbb{R}^{2n}} \|B_j\Psi_{Zh}\|^2 dZ = (2\pi h)^{-n}\int_{\mathbb{R}^{2n}} < B_j^\star B_j\Psi_{Zh}, \Psi_{Zh} > \ dZ$$

$$= \mathrm{Tr}(B_j^\star B_j) = \|B_j\|^2_{\mathcal{L}^2(\mathcal{H})}$$

where $\|B_j\|_{\mathcal{L}^2(\mathcal{H})}$ is the Hilbert-Schmidt norm of B_j. Therefore,

$$I_h \leq (2\pi)^{-n}\|G\|_{L^1(\mathbb{R}^{2n})}\ \|B_1\|_{\mathcal{L}^2(\mathcal{H})}\ \|B_2\|_{\mathcal{L}^2(\mathcal{H})}.$$

Taking the infimum over all A written as $A = B_1B_2$ we then obtain (4.12).

□

Let us finally recall the following proposition even if it is standard.

Proposition 4.4. *The Wick symbol $\sigma_h^{wick}(A)$ of an operator A is related to its Weyl symbol $\sigma_h^{weyl}(A)$ by*

$$\sigma_h^{wick}(A) = e^{\frac{h}{4}\Delta}\sigma_h^{weyl}(A) \tag{4.13}$$

where Δ is the Laplacian on $\mathbb{R}^{2n}$.

Indeed, setting $F_h = \sigma_h^{weyl}(A)$, the expression in definition (1.7) for the Weyl calculus may be written as:

$$A = (\pi h)^{-n} \int_{\mathbb{R}^{2n}} F_h(Y) \Sigma_{Yh} dY, \tag{4.14}$$

where, for all $Y = (y, \eta)$ in $\mathbb{R}^{2n}$, Σ_{Yh} is the operator ("symmetry operator") defined by,

$$(\Sigma_{Yh} f)(u) = e^{\frac{2i}{h}(u-y)\xi} f(2y - u) \qquad Y = (y, \eta) \in \mathbb{R}^{2n}. \tag{4.15}$$

A direct computation shows that:

$$\sigma_h^{wick}(\Sigma_{Yh})(X) = < \Sigma_{Yh} \Psi_{Xh}, \Psi_{Xh} > = e^{-\frac{|X-Y|^2}{h}}. \tag{4.16}$$

Equality (4.13) then follows.

5. Pseudo-differential approximation.

The class of operators having a Weyl symbol in $W^{\infty 1}(\mathbb{R}^{2n})$ (introduced by C. Rondeaux) is dense in the set of trace class operators similarly to the fact that $W^{\infty 1}(\mathbb{R}^n)$ is dense in $L^1(\mathbb{R}^n)$. The approximation process has a strong connection with convolutions and may probably be also applied to Schatten's classes. This process is often employed in representation theory. However, as for a function in $L^\infty(\mathbb{R}^n)$ needs to be continuous in order to be in the closure of $W^{\infty\infty}(\mathbb{R}^n)$, a bounded operator needs additional hypotheses in order to be in the closure of the class of Calderon-Vaillancourt for operators.

For all $X = (x, \xi)$ in $\mathbb{R}^n$ and for all $h > 0$ let $W_{x,\xi,h}$ be the operator defined by

$$(W_{X,h} f) = (W_{x,\xi,h} f)(u) = f(u - x) e^{\frac{i}{h} u.\xi - \frac{i}{2h} x.\xi} \tag{5.1}$$

for all $f \in L^2(\mathbb{R}^n)$. It is a common representation of the group of Heisenberg. Thus, the coherent state Ψ_{Xh} verifies,

$$\Psi_{X,h} = W_{X,h} \Psi_{0,h} \tag{5.2}$$

We have, for all X and Y in $\mathbb{R}^{2n}$

$$W_{X,h} W_{Y,h} = e^{\frac{i}{2h}\sigma(X,Y)} W_{X+Y,h} \tag{5.3}$$

where σ is the symplectic form $\sigma((x, \xi), (y, \eta)) = y.\xi - x.\eta$. For all operators A in $\mathcal{L}(\mathcal{H})$ and for all $h > 0$ let us define,

$$\mathcal{T}_h A = (\pi h)^{-n} \int_{\mathbb{R}^{2n}} e^{-\frac{|X|^2}{h}} W_{X,h} A W_{X,h}^\star \, dX \tag{5.4}$$

We begin with the case of bounded and trace class operators satisfying some hypotheses involving their commutators with position and momentum operators.

Theorem 5.1. *a) We have:*

$$\|\mathcal{T}_h A\|_{\mathcal{L}(\mathcal{H})} \leq \|A\|_{\mathcal{L}(\mathcal{H})} \tag{5.5}$$

for all operators A in $\mathcal{L}(\mathcal{H})$ and for all $h > 0$.
b) When the commutators $[P_j(h), A]$ and $[Q_j(h), A]$ are bounded operators we have:

$$\|A - \mathcal{T}_h A\|_{\mathcal{L}(\mathcal{H})} \leq \frac{C}{\sqrt{h}} \sum_{j=1}^n \|[P_j(h), A]\|_{\mathcal{L}(\mathcal{H})} + \|[Q_j(h), A]\|_{\mathcal{L}(\mathcal{H})}. \tag{5.6}$$

c) When the operator A is trace class together with the commutators $[P_j(h), A]$ and $[Q_j(h), A]$, we have:

$$\|A - \mathcal{T}_h A\|_{\mathcal{L}^1(\mathcal{H})} \leq \frac{C}{\sqrt{h}} \sum_{j=1}^n \|[P_j(h), A]\|_{\mathcal{L}^1(\mathcal{H})} + \|[Q_j(h), A]\|_{\mathcal{L}^1(\mathcal{H})}. \tag{5.7}$$

d) The Wick symbol of the operators A and $\mathcal{T}_h A$ are related with:

$$\sigma_h^{wick}(\mathcal{T}_h A) = e^{\frac{h}{4}\Delta} \sigma_h^{wick}(A). \tag{5.8}$$

The Weyl symbol of $\mathcal{T}_h A$ is equal to the Wick symbol of A.

Proof. Point a) is clear since W_{Xh} is unitary. For any θ in $[0,1]$ define:

$$T(\theta, h)A = (\pi h)^{-n} \int_{\mathbb{R}^{2n}} e^{-\frac{|X|^2}{h}} W_{\theta X, h} A W^\star_{\theta X, h}\, dX.$$

Thus $T(1,h)A = T_h A$ and $T(0,h)A = A$. We verify that:

$$\frac{\partial}{\partial \theta} W_{\theta X, h} A W^\star_{\theta X, h} = \frac{i}{h} \sum_{j=1}^n \Big[x_j W_{\theta X, h} [P_j(h), A] W^\star_{\theta X, h} - \xi_j W_{\theta X, h} [Q_j(h), A] W^\star_{\theta X, h} \Big].$$

Consequently:

$$\|A - \mathcal{T}_h A\|_{\mathcal{L}(\mathcal{H})} \leq \frac{1}{h} \sum_{j=1}^n (\pi h)^{-n} \int_{\mathbb{R}^{2n} \times [0,1]} e^{-\frac{|X|^2}{h}} \Big[|x_j|\ \|[P_j(h), A]\|_{\mathcal{L}(\mathcal{H})} + |\xi_j|\ \|[Q_j(h), A]\|_{\mathcal{L}(\mathcal{H})} \Big] dx d\xi d\theta$$

$$\leq \frac{C}{\sqrt{h}} \sum_{j=1}^n \|(ad P_j(h))A\|_{\mathcal{L}(\mathcal{H})} + \|(ad Q_j(h))A\|_{\mathcal{L}(\mathcal{H})}$$

proving point b) and also point c) with straightforward modifications. For the point d) we see that:

$$\sigma_h^{wick}(\mathcal{T}_h A)(X) = < (\mathcal{T}_h A)\Psi_{Xh}, \Psi_{Xh} > = < (\mathcal{T}_h A) W_{X,h} \Psi_{0h}, W_{X,h} \Psi_{0h} >$$

$$= (\pi h)^{-n} \int_{\mathbb{R}^{2n}} e^{-\frac{|Y|^2}{h}} < W_{Y,h} A W^\star_{Y,h} W_{X,h} \Psi_{0h}, W_{X,h} \Psi_{0h} > \ dY$$

$$= (\pi h)^{-n} \int_{\mathbb{R}^{2n}} e^{-\frac{|Y|^2}{h}} < A W_{X-Y,h} \Psi_{0h}, W_{X-Y,h} \Psi_{0h} > dY.$$

We have used here (5.3). Consequently,

$$\sigma_h^{wick}(\mathcal{T}_h A)(X) = (\pi h)^{-n} \int_{\mathbb{R}^{2n}} e^{-\frac{|Y|^2}{h}} \sigma_h^{wick}(A)(X - Y) dY$$

which is (5.8). According to proposition 4.4 we also have:

$$\sigma_h^{wick}(\mathcal{T}_h A) = e^{\frac{h}{4}\Delta} \sigma_h^{weyl}(\mathcal{T}_h A).$$

Since the operator $e^{\frac{h}{4}\Delta}$ is one to one we then deduce as it is mentioned,

$$\sigma_h^{weyl}(\mathcal{T}_h A) = \sigma_h^{wick}(A).$$

$\square$

Next we consider the case of trace class operators without additional assumptions. The result below does not have any counterpart in the case of bounded operators.

Theorem 5.2. *The space of operators written as $OP_h^{weyl}(F)$ with F in $W^{\infty 1}(\mathbb{R}^{2n})$ is dense in the space $\mathcal{L}^1(\mathcal{H})$ of trace class operators.*

Proof. For this purpose, we modify the approximation process and we set:

$$\mathcal{T}'_\lambda A = (\pi\lambda)^{-n} \int_{\mathbb{R}^{2n}} e^{-\frac{|X|^2}{\lambda}} W_{X,1} A W^\star_{X,1}\ dX$$

for all $\lambda > 0$ and for all trace class operators A. Let us show that:

$$\lim_{\lambda\to 0} \|\mathcal{T}'_\lambda(A) - A\|_{\mathcal{L}^1(\mathcal{H})} = 0 \tag{5.9}$$

for all trace class operators A. Since we clearly have

$$A = (\pi\lambda)^{-n} \int_{\mathbb{R}^{2n}} e^{-\frac{|X|^2}{\lambda}} A\ dX$$

then we see that:

$$\|\mathcal{T}'_\lambda(A) - A\|_{\mathcal{L}^1(\mathcal{H})} \leq (\pi\lambda)^{-n} \int_{|X|<\delta} e^{-\frac{|X|^2}{\lambda}} \|W_{X,h} A W^\star_{X,h} - A\|_{\mathcal{L}^1(\mathcal{H})} + ...$$

$$... + (\pi\lambda)^{-n} \int_{|X|>\delta} e^{-\frac{|X|^2}{\lambda}} \Big[\|W_{X,\lambda} A W^\star_{X,h}\|_{\mathcal{L}^1(\mathcal{H})} + \|A\|_{\mathcal{L}^1(\mathcal{H})}\Big] dX$$

for all $\delta > 0$ and for all $\lambda > 0$. For all trace class operators A and for all $\varepsilon > 0$ there exists $\delta > 0$ such that:

$$|X| < \delta, \Longrightarrow \|W_{X,1} A W^\star_{X,1} - A\|_{\mathcal{L}^1(\mathcal{H})} < \varepsilon.$$

Indeed, this property is first verified when A is of the form $f \to < f, \varphi > \psi$ with φ and ψ in $\mathcal{S}(\mathbb{R}^n)$, it is next derived by density for finite-rank operators and then, by density again for trace class operators. Besides, $\delta > 0$ being fixed, we have:

$$\lim_{\lambda\to 0} (\pi\lambda)^{-n} \int_{|X|>\delta} e^{-\frac{|X|^2}{\lambda}} \Big[\|W_{X,1} A W^\star_{X,1}\|_{\mathcal{L}^1(\mathcal{H})} + \|A\|_{\mathcal{L}^1(\mathcal{H})}\Big] dX = 0.$$

The limit in (5.9) is then easily obtained. From (5.3), for all X in $\mathbb{R}^{2n}$ we have:

$$W_{X,1} \mathcal{T}'_\lambda(A) W^\star_{X,1} = (\pi\lambda)^{-n} \int_{\mathbb{R}^{2n}} e^{-\frac{|Y|^2}{\lambda}} W_{X+Y,1} A W^\star_{X+Y,1}\ dY$$

$$= (\pi\lambda)^{-n} \int_{\mathbb{R}^{2n}} e^{-\frac{|X-Z|^2}{\lambda}} W_{Z,1} A W^\star_{Z,1}\ dZ.$$

Consequently, for all $\lambda > 0$, the mapping $X \to W_{X,1} \mathcal{T}'_\lambda(A) W^\star_{X,1}$ is C^∞ from $\mathbb{R}^{2n}$ into $\mathcal{L}^1(\mathcal{H})$. We see, setting $X = (x, \xi)$ as the variable of $\mathbb{R}^{2n}$,

$$\frac{\partial}{\partial x_j} W_{X,1} \mathcal{T}'_\lambda(A) W^\star_{X,1} = -W_{X,1} \Big[P_j(1), \mathcal{T}'_\lambda(A)\Big] W^\star_{X,1}$$

$$\frac{\partial}{\partial \xi_j} W_{X,1} \mathcal{T}'_\lambda(A) W^\star_{X,1} = W_{X,1} \Big[Q_j(1), \mathcal{T}'_\lambda(A)\Big] W^\star_{X,1}$$

where $P_j(1)$ is the operator of differentiation with respect to u_j and $Q_j(1)$ is the multiplication operator by u_j. Consequently, all order iterated commutators $\mathcal{T}'_\lambda(A)$ with the position and momentum operators $P_j(1)$ and $Q_j(1)$ are trace class. From the result of characterization of C. Rondeaux [R] (the analogous one of Beals's characterization for trace class operators and recalled in the first part of this work) it follows that $\mathcal{T}'_\lambda(A)$ is written as $Op_1^{weyl}(F_\lambda)$ with F_λ in $W^{\infty 1}(\mathbb{R}^{2n})$ for all $\lambda > 0$.

6. Proof of theorem 1.1.

Let A be an operator in $\mathcal{L}(\mathcal{H})$ satisfying the assumptions in theorem 1.1. Set $F_h(X) = \sigma_h^{wick}(A)(X)$. This function is C^∞ from proposition 4.1. Denoting by φ_t the Hamiltonian flow associated to the function $H(x,\xi) = |\xi|^2 + V(x)$, we shall use the following function and operators:

$$w_h(X,t) = F_h(\varphi_t(X)) \qquad\qquad C_h(t) = Op_h^{weyl}(w_h(.,t)). \tag{6.1}$$

We shall also use the operator $\mathcal{T}_h A$ appearing in section 5 and the following operator:

$$B_h(t) = e^{i\frac{t}{h}\widehat{H}_h}\mathcal{T}_h(A)e^{-i\frac{t}{h}\widehat{H}_h}. \tag{6.2}$$

We shall compare Wick symbols of the operators $A_h(t)$, $B_h(t)$ and $C_h(t)$ and then compare the Wick symbol of $C(t,h)$ with the function $w_h(.,t)$. This is accomplished in the three steps below.

First step. We have, from theorem 5.1,

$$\|\sigma_h^{wick}(A_h(t) - B_h(t))\|_{L^\infty(\mathbb{R}^{2n})} \leq \|A_h(t) - B_h(t)\|_{\mathcal{L}(\mathcal{H})} = \|A - T_h(A)\|_{\mathcal{L}(\mathcal{H})} \tag{6.3}$$

$$... \leq C\sqrt{h} I_h^\infty(A)$$

where $I_h^\infty(A)$ is defined in (1.13).

Second step. The comparison of $B_h(t)$ and $C_h(t)$ comes from Egorov's theorem. Nevertheless this requires some precisions due to unusual estimates satisfied by the derivatives of $w_h(.,t)$ that we first need to specify. Since $w_h(.,0) = \sigma_h^{wick}(A)$ we deduce that:

$$\frac{\partial w_h(.,0)}{\partial x_j} = \frac{i}{h}\sigma_h^{wick}([P_j(h), A]) \qquad\qquad \frac{\partial w_h(.,0)}{\partial \xi_j} = -\frac{i}{h}\sigma_h^{wick}([Q_j(h), A]).$$

Applying proposition 4.1 to the above commutators we see when $k \geq 1$ that:

$$\|\nabla^k w_h(.,0)\|_{L^\infty(\mathbb{R}^{2n})} \leq C_{\alpha\beta} h^{1-(k+1)/2} I_h^\infty(A).$$

The derivatives of order ≥ 1 of the Hamiltonian flow φ_t associated to the symbol $H(x,\xi) = |\xi|^2 + V(x)$ are bounded in R^{2n} with a bound equaling to $\mathcal{O}(1+t^2)$. Then there exists $M_k(t)$ such that:

$$\|\nabla^k w_h(.,t)\|_{L^\infty(\mathbb{R}^{2n})} \leq M_k(t) h^{1-(k+1)/2} I_h^\infty(A). \tag{6.4}$$

The operators $B_h(t)$ and $C_h(t)$ satisfy:

$$-ih\frac{\partial B_h(t)}{\partial t} = [\widehat{H}_h, B(t,h)] \tag{6.5}$$

$$-ih\frac{\partial C_h(t)}{\partial t} = -ihOp_h^{weyl}(\partial_t w_h(.,t)) = -ihOp_h^{weyl}(\{H, w_h(.,t)\}).$$

From a standard result on the Weyl calculus recalled in proposition 3.2 of [AKN] (first part of this work), for all functions F and G in $W^{\infty\infty}(\mathbb{R}^{2n})$, the operator $\widehat{R}_h^{(2)}(F,G)$ defined by:

$$[Op_h^{weyl}(F), Op_h^{weyl}(F)] = \frac{h}{i}Op_h^{weyl}(\{F,G\}) + \widehat{R}_h^{(2)}(F,G)$$

satisfies the following estimate:

$$\|\widehat{R}_h^{(2)}(F,G)\|_{\mathcal{L}(\mathcal{H})} \leq C \sum_{\substack{j\geq 2, k\geq 2\\ 4\leq j+k\leq 6n+8}} h^{(j+k)/2} \|\nabla^j F\|_{L^\infty(\mathbb{R}^{2n})} \ \|\nabla^k G\|_{L^\infty(\mathbb{R}^{2n})}. \tag{6.6}$$

With these notations, one may write:

$$-ih\frac{\partial C_h(t)}{\partial t} - [\widehat{H}_h, C_h(t)] = \widehat{R}_h^{(2)}(H, w_h(.,t)). \tag{6.7}$$

Note that $\widehat{R}_h^{(2)}(\Delta, w_h(.,t)) = 0$ and consequently

$$\widehat{R}_h^{(2)}(H, w_h(.,t)) = \widehat{R}_h^{(2)}(V, w_h(.,t)).$$

We then may apply inequality (6.6) with the functions $F = V$ and $G = w_h(.,t)$. The inequality (6.6), those in (6.4) which are verified by $w_h(.,t)$, and the fact that all derivatives of V are bounded allows us to write:

$$\|\widehat{R}_h^{(2)}(H, G_h(.,t))\|_{\mathcal{L}(\mathcal{H})} \leq M(t)\ h^{3/2}\ I_h^\infty(A). \tag{6.8}$$

From theorem 5.1, the operator $\mathcal{T}_h A$ appearing in section 5 has a Weyl symbol equal to the Wick symbol of A. Consequently, the Weyl symbol of $B_h(0) = \mathcal{T}_h(A)$ and the one of $C_h(0)$ which is $F_h = \sigma_h^{wick}(A)$ are equal. Thus,

$$B_h(0) = C_h(0). \tag{6.9}$$

From (6.5), (6.7) and (6.9), Duhamel's principle implies:

$$ih[B_h(t) - C_h(t)] = \int_0^t e^{i\frac{t-s}{h}\widehat{H}_h}\ \widehat{R}_h^{(2)}(H, G_h(.,t))\ e^{-i\frac{t-s}{h}\widehat{H}_h}\ ds.$$

Consequently, when $t > 0$:

$$\|B_h(t) - C_h(t)\|_{\mathcal{L}(\mathcal{H})} \leq \frac{1}{h}\int_0^t \|\widehat{R}_h^{(2)}(H, G_h(.,s))\|_{\mathcal{L}(\mathcal{H})} ds.$$

We then deduce that:

$$\|\sigma_h^{wick}\Big(B_h(t) - C_h(t)\Big)\|_{L^\infty(\mathbb{R}^{2n})} \leq \|B_h(t) - C_h(t)\|_{\mathcal{L}(\mathcal{H})} \leq M(t)\sqrt{h}\ I_h^\infty(A). \tag{6.10}$$

Third step. From proposition 4.4,

$$\sigma_h^{wick}((C_h(t)) = e^{\frac{h}{4}\Delta}\sigma_h^{weyl}(C_h(t)) = e^{\frac{h}{4}\Delta} w_h(.,t).$$

Then

$$\|\sigma_h^{wick}((C_h(t)) - w_h(.,t)\|_{L^\infty(\mathbb{R}^{2n})} \leq \frac{h}{4}\int_0^1 \|\Delta e^{\frac{\theta h}{4}\Delta} w_h(.,t)\|_{L^\infty(\mathbb{R}^{2n})} \leq \|\Delta w_h(.,t)\|_{L^\infty(\mathbb{R}^{2n})}.$$

In view of the estimates (6.4) satisfied by $w_h(.,t)$, we obtain:

$$\|\sigma_h^{wick}(C_h(t)) - w_h(.,t)\|_{L^\infty(\mathbb{R}^{2n})} \leq M(t)\sqrt{h} I_h^\infty(A). \tag{6.11}$$

Since $w_h(.,t) = \Big(\sigma_h^{wick}(A)\Big) \circ \varphi_t$, then inequality (1.14) in theorem 1.1 arises from (6.3), (6.10) and (6.11).

7. Proof of theorem 2.1.

Let $\rho_h(t)$ be a family of solutions to the equation (TDHF) (2.1), satisfying the hypotheses of theorem 2.1. Let $u_h(.,t)$ be the function defined in (2.3). Let $v_h(.,t)$ be the solution to Vlasov equation (2.5) such that $v_h(.,0) = u_h(.,0)$. We shall use the functions $V_q(.,\rho_h(t))$ and $V_{cl}(.,v_h(.,t))$ defined in (2.2) and (2.7) respectively. We shall also use the following functions

$$H_h^{HF}(x,\xi,t) = |\xi|^2 + V_q(x,\rho_h(t)) \qquad H_h^{VL}(x,\xi,t) = |\xi|^2 + V_{cl}(x,v_h(.,t)) \tag{7.1}$$

and the associated operators through the Weyl calculus, namely:

$$\widehat{H}_h^{HF} = -h^2\Delta + V_q(.,\rho_h(t)) \qquad \widehat{H}_h^{VL} = -h^2\Delta + V_{cl}(x,v_h(.,t)), \tag{7.2}$$

by using the same notation for the function and the corresponding multiplication operator. We shall denote by $w_h(X,t)$ the solution to

$$\frac{\partial w_h}{\partial t}(.,t) = \{H_h^{HF}(.,t), w_h(.,t)\}, \tag{7.3}$$

such that

$$w_h(.,0) = v_h(.,0) = u_h(.,0). \tag{7.4}$$

In order to compare $v_h(.,t)$ with $w_h(.,t)$ we note that the Vlasov equation (2.5) is written as

$$\frac{\partial v_h}{\partial t}(.,t) = \{H_h^{VL}(.,t), v_h(.,t)\}. \tag{7.5}$$

We shall use the operator $B_h(t)$ solution to

$$ih\frac{dB_h(t)}{dt} = [\widehat{H}_h^{HF}(t), B_h(t)] \qquad B_h(0) = \mathcal{T}_h(\rho_h(0)), \tag{7.6}$$

where $\mathcal{T}_h$ is the mapping used in section 5. Finally, we shall also use the following operators:

$$C_h(t) = (2\pi h)^n Op_h^{weyl}(w_h(.,t)) \qquad D_h(t) = (2\pi h)^n Op_h^{weyl}(v_h(.,t)). \tag{7.7}$$

According to the point d) in theorem 5.1, we have

$$\sigma_h^{weyl}(B_h(0)) = \sigma_h^{weyl}\Big(\mathcal{T}_h(\rho_h(0))\Big) = \sigma_h^{wick}(\rho_h(0)) = (2\pi h)^n u_h(.,0). \tag{7.8}$$

Consequently,

$$B_h(0) = C_h(0) = D_h(0) \tag{7.9}$$

Theorem 2.1 is a consequence of the comparison between the Wick symbol of the operators $\rho_h(t)$ and $B_h(t)$, between those of $B_h(t)$ and $C_h(t)$, between those of $C_h(t)$ and $D_h(t)$, and finally between the Wick symbol of $D_h(t)$ and the function $v_h(.,t)$. Each of these comparisons shall be written using the expression $I_h^{tr}(\rho_h(0))$ defined in (2.8), and shall correspond to one step of the proof, but before that, we need three more lemmata.

Lemma 7.1. *Let $\rho_h(t)$ be a family of solutions to the (TDHF) equation satisfying the assumptions in theorem 2.1. Let $v_h(.,t)$ be the function defined above. Then, for all integer numbers $k \geq 0$ we have*

$$\|\nabla^k v_h(.,t)\|_{L^1(\mathbb{R}^{2n})} \leq C_k(t) h^{-k/2} \|\rho_h(0)\|_{\mathcal{L}^1(\mathcal{H})} \tag{7.10}$$

and for all integer numbers $k \geq 1$

$$\|\nabla^k v_h(.,t)\|_{L^1(\mathbb{R}^{2n})} \leq C_k(t) h^{-(k-1)/2} I_h^{tr}(\rho_h(0)). \tag{7.11}$$

These estimates remain valid when replacing the function $v_h(.,t)$ by the function $w_h(.,t)$.

Proof of the lemma. Since we have (7.4) for $t=0$, then the estimates (7.10) and (7.11) when $t=0$ come from proposition 4.2 applied with the operator $\rho_h(0)$ (for (7.10)) and with the commutators $[P_j(h),\rho_h(0)]$ and $[Q_j(h),\rho_h(0)]$ (for (7.11)). Since the potentials V and W are in $W^{\infty\infty}(\mathbb{R}^n)$, then the functions $V_q(.,\rho_h(t))$ and $V_{cl}(.,v_h(.,t))$ are uniformly bounded together with all of their derivatives. Consequently, the estimates satisfied at $t=0$ by $v_h(.,0)=w_h(.,0)$ remain valid along the Hamiltonian flows associated to the two symbols $H_h^{HF}(.,t)$ and $H_h^{VL}(.,t)$. Thus, the estimates (7.10) and (7.11) remain valid for all t for the function $v_h(.,t)$ and the function $w_h(.,t)$.

Lemma 7.2 *If W is a function in $W^{\infty\infty}(\mathbb{R}^n)$, if we denote by W_x the multiplication by $y\to W(x-y)$ and if A is trace class, then*

$$e^{\frac{h}{4}\Delta_x}Tr(W_x\circ A)=(2\pi h)^{-n}\int_{\mathbb{R}^{2n}}W(x-y)\sigma_h^{wick}(A)(y,\eta)dyd\eta. \tag{7.12}$$

Proof of the lemma. From (3.2), if W is as in the lemma and if $A=Op_h^{weyl}(F)$ with F in $W^{\infty 1}(\mathbb{R}^{2n})$, then we have:

$$Tr(W_x\circ A)=(2\pi h)^{-n}\int_{\mathbb{R}^{2n}}W(x-y)\sigma_h^{weyl}(A)(y,\eta)dyd\eta$$

and then

$$e^{\frac{h}{4}\Delta_x}Tr(W_x\circ A)=(2\pi h)^{-n}\int_{\mathbb{R}^{2n}}W(x-y)e^{\frac{h}{4}\Delta_x}\sigma_h^{weyl}(A)(y,\eta)dyd\eta.$$

Besides

$$\int_{\mathbb{R}^{2n}}W(x-y)\ (e^{\frac{h}{4}\Delta_\eta}-I)\ \sigma_h^{weyl}(A)(y,\eta)dyd\eta=0,$$

and taking into account proposition 4.4 we deduce (7.12). Suppose now that A is an arbitrarily given trace class operator. Then theorem 5.2 shows that there exists a sequence of operators A_j, written as $A_j=Op_h^{weyl}(F_j)$ with F_j in $W^{\infty 1}(\mathbb{R}^{2n})$ converging to A in $\mathcal{L}^1(\mathcal{H})$, ($h>0$ being fixed). Equality (7.12) valid for all the A_j is also true for A when taking the limit while using proposition 4.2. □

Lemma 7.3. *With the above notations, we have:*

$$\|v_h(.,t)-w_h(.,t)\|_{L^1(\mathbb{R}^{2n})}\le C(t)I_h^{tr}(\rho_h(0))\left[h+\int_{[0,t]}\|v_h(.,s)-u_h(.,s)\|_{L^1(\mathbb{R}^{2n})}ds\right]. \tag{7.13}$$

Proof of the lemma. We deduce from (7.3) and (7.5) that:

$$\frac{\partial(v_h-w_h)}{\partial t}(.,t)=\{H_h^{HF}(.,t),(v_h(.,t)-w_h(.,t))\}+\{(H_h^{HF}(.,t)-H_h^{VL}(.,t)),v_h(.,t)\}$$

From Duhamel's principle, since $v_h(.,0)-w_h(.,0)=0$ and since the Hamiltonian flow associated to the function $H_h^{HF}(.,t)$ preserves the norm of $L^1(\mathbb{R}^{2n})$, we obtain

$$\|v_h(.,t)-w_h(.,t)\|_{L^1(\mathbb{R}^{2n})}\le\int_{[0,t]}\|\{H_h^{HF}(.,s)-H_h^{VL}(.,s)\ ,\ v_h(.,s)\}\|_{L^1(\mathbb{R}^{2n})}ds.$$

We have:

$$H_h^{HF}(.,s)-H_h^{VL}(.,s)=(I-e^{\frac{h}{4}\Delta_x})Tr(W_x\circ\rho_h(t))+e^{\frac{h}{4}\Delta_x}Tr(W_x\circ\rho_h(t))-\int_{\mathbb{R}^{2n}}W(x-y)v_h(y,\eta,t)dyd\eta.$$

From lemma 7.2, we have:

$$e^{\frac{h}{4}\Delta_x} Tr(W_x \circ \rho_h(t)) = \int_{\mathbb{R}^{2n}} W(x-y)\ u_h(y,\eta,t) dy d\eta.$$

We then deduce

$$H_h^{HF}(x,\xi,s) - H_h^{VL}(x,\xi,s) = (I - e^{\frac{h}{4}\Delta_x}) Tr(W_x \circ \rho_h(t)) + ...$$
$$... + \int_{\mathbb{R}^{2n}} W(x-y)\ \Big(u_h(y,\eta,t) - v_h(y,\eta,t)\Big) dy d\eta.$$

In view of the preceding points,

$$\|v_h(.,t) - w_h(.,t)\|_{L^1(\mathbb{R}^{2n})} \leq C \int_{[0,t]} \|\nabla v_h(.,s)\}\|_{L^1(\mathbb{R}^{2n})} \Big[h + \|u_h(.,s) - v_h(.,s)\|_{L^1(\mathbb{R}^{2n})} \Big] ds.$$

From lemma 7.1 (with $k=1$) we then deduce (7.13).

End of the proof of theorem 2.1. First step. With the above notations, (TDHF) equation is written as:

$$ih \frac{d\rho_h(t)}{dt} = [\widehat{H}_h^{HF}(t), \rho_h(t)].$$

We consequently have

$$ih \frac{d(\rho_h(t) - B_h(t))}{dt} = [\widehat{H}_h^{HF}(t), (\rho_h(t) - B_h(t))].$$

Since the propagator associated to this equation preserves the trace norm, and since $B_h(0) = \mathcal{T}_h(\rho_h(0))$, we then deduce

$$\|\rho_h(t) - B_h(t)\|_{\mathcal{L}^1(\mathcal{H})} \leq \|\rho_h(0) - \mathcal{T}_h(\rho_h(0))\|_{\mathcal{L}^1(\mathcal{H})}.$$

Consequently, from the proposition 4.2 (with $m=0$) and theorem 5.1 (point c)),

$$(2\pi h)^{-n} \|\sigma_h^{wick}\Big(\rho_h(t) - B_h(t)\Big)\|_{L^1(\mathbb{R}^{2n})} \leq \|\rho_h(0) - \mathcal{T}_h(\rho_h(0))\|_{\mathcal{L}^1(\mathcal{H})} \leq C\sqrt{h} I_h^{tr}(\rho_h(0)). \tag{7.14}$$

Second step. We shall bound in norm $B_h(t) - C_h(t)$ and in this aim we shall show that $B_h(t)$ and $C_h(t)$ verify similar equations. The operator $B_h(t)$ verifies (7.6) whereas

$$ih \frac{dC_h(t)}{dt} = ih(2\pi h)^n OP_h^{weyl}(\{H_h^{HF}(.,t), w_h(.,t)\}).$$

With the notations of section 3 in [AKN] we have:

$$[OP_h^{weyl}(H_h^{HF}(.,t)), OP_h^{weyl}(w_h(.,t))] = \frac{h}{i} OP_h^{weyl}(\{H_h^{HF}(.,t), w_h(.,t)\}) + \widehat{R}_h^{(2)}(H_h^{HF}(.,t), w_h(.,t)).$$

Consequently,

$$ih \frac{dC_h(t)}{dt} - [\widehat{H}_h^{HF}(t), C_h(t)] = (2\pi h)^n \widehat{R}_h^{(2)}(H_h^{HF}(.,t), w_h(.,t)). \tag{7.15}$$

We know that $R_h^{(2)}(F,G) = 0$ for all function G when $F(x,\xi) = |\xi|^2$. We can then replace $H_h^{HF}(.,t)$ by $V_q(.,\rho_h(t))$ in the right hand-side of (7.15). By combining (7.15) with equation (7.6) verified by $B_h(t)$ and using Duhamel's principle and (7.4), we obtain

$$\|B_h(t) - C_h(t)\|_{\mathcal{L}^1(\mathcal{H})} \leq \frac{1}{h}(2\pi h)^n \int_{[0,t]} \|\widehat{R}_h^{(2)}(V_q(.,\rho_h(s)), w_h(.,s))\|_{\mathcal{L}^1(\mathcal{H})} ds.$$

From theorem 3.1 of [AKN] applied with $N=2$, $F=V_q(.,\rho_h(s))$, $G=w_h(.,s)$, $p=\infty$, $q=1$, we have

$$\|\widehat{R}_h^{(2)}(V_q(.,\rho_h(s)),w_h(.,s))\|_{\mathcal{L}^1(\mathcal{H})} \leq Ch^{-n} \sum_{\substack{\alpha+\beta\leq 6n+8\\ \alpha\geq 2,\beta\geq 2}} h^{(\alpha+\beta)/2} \|\nabla^\alpha V_q(.,\rho_h(s))\|_{L^\infty(\mathbb{R}^n)} \|\nabla^\beta w_h(.,s)\|_{L^1(\mathbb{R}^{2n})}.$$

Since the potentials V and W are in $W^{\infty\infty}(\mathbb{R}^n)$ and since the $L^1(\mathbb{R}^{2n})$ norm of $w_h(.,s)$ is bounded (lemma 7.1) then the derivatives of all order of $V_q(.,\rho_h(s))$ are bounded. For $\beta\geq 1$ the function $\nabla^\beta w_h(.,s)$ verifies the estimates (7.11) of lemma 7.1. Consequently, when $h\in(0,1]$,

$$\|\widehat{R}_h^{(2)}(V_q(.,\rho_h(s)),w_h(.,s))\|_{\mathcal{L}^1(\mathcal{H})} \leq C(s)h^{3/2} I_h^{tr}(\rho_h(0)).$$

Consequently,

$$\|B_h(t)-C_h(t)\|_{\mathcal{L}^1(\mathcal{H})} \leq C(t)\sqrt{h} I_h^{tr}(\rho_h(0)).$$

We then deduce (from the Proposition 4.2 with $m=0$) that:

$$(2\pi h)^{-n} \left\|\sigma_h^{wick}\big(B_h(t)-C_h(t)\big)\right\|_{L^1(\mathbb{R}^{2n})} \leq C(t)\sqrt{h} I_h^{tr}(\rho_h(0)). \tag{7.16}$$

Third step. From the proposition 4.4, we have

$$(2\pi h)^{-n}\|\sigma_h^{wick}(C_h(t)-D_h(t))\|_{L^1(\mathbb{R}^{2n})} \leq \|e^{\frac{h}{4}\Delta}(v_h(.,t)-w_h(.,t)\|_{L^1(\mathbb{R}^{2n})} \leq \|(v_h(.,t)-w_h(.,t)\|_{L^1(\mathbb{R}^{2n})}.$$

Then, from lemma 7.2,

$$(2\pi h)^{-n}\|\sigma_h^{wick}(C_h(t)-D_h(t))\|_{L^1(\mathbb{R}^{2n})} \leq CI_h(\rho_h(0)) \left[h + \int_{[0,t]} \|u_h(.,s)-v_h(.,s)\|_{L^1(\mathbb{R}^{2n})} ds \right]. \tag{7.17}$$

Fourth step. From proposition 4.4 we have

$$(2\pi h)^{-n}\sigma_h^{wick}(D_h(t)) = (2\pi h)^{-n} e^{\frac{h}{4}\Delta}\sigma_h^{weyl}(D_h(t)) = e^{\frac{h}{4}\Delta} v_h(.,t).$$

Consequently, from the lemma 7.1 with $k=2$, we obtain

$$\|v_h(.,t)-(2\pi h)^{-n}\sigma_h^{wick}(D_h(t)\|_{L^1(\mathbb{R}^{2n})} \leq \|(e^{\frac{h}{4}\Delta}-I)v_h(.,t)\|_{L^1(\mathbb{R}^{2n})} \leq ...$$

$$... \leq Ch\|\nabla^2 v_h(.,t)\|_{L^1(\mathbb{R}^{2n})} \leq C(t)\sqrt{h} I_h^{tr}(\rho_h(0)). \tag{7.18}$$

Since $u_h(.,t)$ is defined by (2.3), we obtain from estimates (7.14), (7.16), (7.17) and (7.18) obtained in the four steps that:

$$\|u_h(.,t)-v_h(.,t)\|_{L^1(\mathbb{R}^{2n})} \leq C(t) I_h^{tr}(\rho_h(0)) \left[\sqrt{h} + \int_{[0,t]} \|u_h(.,s)-v_h(.,s)\|_{L^1(\mathbb{R}^{2n})} ds \right].$$

From Gronwall's lemma, we have

$$\|u_h(.,t)-v_h(.,t)\|_{L^1(\mathbb{R}^{2n})} \leq C(t)\sqrt{h} I_h^{tr}(\rho_h(0)) e^{C(t)I_h(\rho_h(0))}$$

if $h\in(0,1]$, with a different constant $C(t)$. Theorem 2.1 is complete.

□

8. Approximative composition of symbols with the Wick calculus.

Being given two continuous operators A and B in $\mathcal{S}(\mathbb{R}^n)$ we can define the Wick symbols $\sigma_h^{wick}(A)$, $\sigma_h^{wick}(B)$ and $\sigma_h^{wick}(A\circ B)$. When one of these two symbols $\sigma_h^{wick}(A)$ or $\sigma_h^{wick}(B)$ is a polynomial function, we can express $\sigma_h^{wick}(A\circ B)$ using an exact formula with the following notations. For any function $F\in C^1(\mathbb{R}^{2n})$ we set

$$\partial_j F = \frac{1}{2}\left[\frac{\partial F}{\partial x_j} - i\frac{\partial F}{\partial \xi_j}\right] \qquad\qquad \overline{\partial}_j F = \frac{1}{2}\left[\frac{\partial F}{\partial x_j} + i\frac{\partial F}{\partial \xi_j}\right].$$

For any multi-index (α,β) we set

$$\partial^\alpha\overline{\partial}^\beta = \partial_1^{\alpha_1}...\partial_n^{\alpha_n}\overline{\partial}_1^{\beta_1}...\overline{\partial}_n^{\beta_n}.$$

When F is a function of several variables in $\mathbb{R}^{2n}$ denoted by W, Y, etc..., we shall write as a subscript the letter giving the variable on which act the operator.

With these notations, if one of the two symbols $\sigma_h^{wick}(A)$ or $\sigma_h^{wick}(B)$ is a polynomial function then we have:

$$\sigma_h^{wick}(A\circ B)(X) = \sum_{|\alpha|<m}\frac{(2h)^\alpha}{\alpha!}\Big[\partial^\alpha\sigma_h^{wick}(A_h)(X)\Big]\ \Big[\overline{\partial}^\alpha\sigma_h^{wick}(B_h)(X)\Big]. \tag{8.1}$$

This formula justifies the terminology since it carries the Wick order of creation and annihilation operators.

In this section, we shall give a similar formula when one of the two operators is trace class while the other one associated through the Weyl calculus has a symbol in $W^{\infty\infty}(\mathbb{R}^{2n})$. In this case, for all integer numbers $m\geq 1$ and for all $h>0$ we shall denote by $R_m(A,B;.;h)$ the function on $\mathbb{R}^{2n}$ defined by the equality

$$\sigma_h^{wick}(A\circ B)(X) = \sum_{|\alpha|<m}\frac{(2h)^\alpha}{\alpha!}\Big[\partial^\alpha\sigma_h^{wick}(A_h)(X)\Big]\ \Big[\overline{\partial}^\alpha\sigma_h^{wick}(B_h)(X)\Big] + R_m(A,B;X;h). \tag{8.2}$$

The main result of this section is the following one.

Theorem 8.1. *We consider two operators A and B such that*
1. The operator A is written as $A = Op_h^{weyl}(F)$ where $F\in W^{\infty\infty}(\mathbb{R}^{2n})$.
2. The operator B is trace class.
Then, for all integer numbers $m\geq 1$ there exists a constant $C_m>0$ (depending only on m and n) such that the functions $R_m(A,B;X;h)$ defined by the equality (8.2) and the analogous function $R_m(B,A;X;h)$ verify:

$$(2\pi h)^{-n}\int_{\mathbb{R}^{2n}}\Big|R_m(A,B;X;h)\Big|\,dX \leq C_{mn}\ \ \|B_h\|_{\mathcal{L}^1(\mathcal{H})}\sum_{\alpha\in E_{mn}} h^{|\alpha|/2}\|\partial^\alpha F\|_{L^\infty(\mathbb{R}^{2n})}, \tag{8.3}$$

where E_{mn} is the following set of multi-indexes,

$$E_{mn} = \{\alpha\in\mathbb{N}^n, \qquad m\leq|\alpha|\leq\sup(m,n+1)\}, \tag{8.4}$$

and similarly for $R_m(B,A;X;h)$.

We shall use the function $S_h(A)$ defined in (4.2) and those which are similarly associated to B and $A\circ B$. We shall refer as $S_h(A)$ for the bi-Wick symbol of A. Using (4.5) we have:

$$\sigma_h^{wick}(A\circ B)(X) = (2\pi h)^{-n}\int_{\mathbb{R}^{2n}}\mathcal{B}_h(X,Y,Y,X)\ S_h(B)(X,Y)\ S_h(A)(Y,X)\ dY. \tag{8.5}$$

The proof of theorem 8.1 relies on a Taylor expansion for the bi-Wick symbol of the operator $A_h = Op_h^{weyl}(F)$ in a neighborhood of the diagonal. It is standard that this bi-symbol is holomorphic in $X = x+i\xi$ and anti-holomorphic in Y. We can give a quick proof. Iterating (4.5) we see that

$$S_h(A)(X,Y) = (2\pi h)^{-n}\int_{\mathbb{R}^{4n}}\mathcal{B}_h(X,U,V,Y)S_h(A)(U,V)dUdV, \tag{8.6}$$

where $\mathcal{B}_h$ is defined in (4.8). Replacing in (4.8) the expression (4.3) giving the scalar product of two coherent states, we obtain an explicit expression of the function $\mathcal{B}_h(X, U, V, Y)$, showing that it is holomorphic in X, anti-holomorphic in Y and $S_h(A)$ inherits therefore of these properties. From these points,

$$S_h(A)(X,Y) = \sum_{\alpha \in \mathbb{N}^n} \frac{(X-Y)^\alpha}{\alpha!} (\partial^\alpha \sigma_h^{wick}(A))(Y) = \sum_{\beta \in \mathbb{N}^n} \frac{(\overline{Y}-\overline{X})^\beta}{\beta!} (\overline{\partial}^\beta \sigma_h^{wick}(A))(X).$$

The first step in the proof of theorem 8.1 is an uniform estimation as h tends to 0 of the remaining terms of order m in the above expansions. Namely,

$$S_h(A)(X,Y) = \sum_{|\alpha|<m} \frac{(X-Y)^\alpha}{\alpha!} (\partial^\alpha \sigma_h^{wick}(A))(Y) + R_m(A; X, Y; h), \tag{8.7}$$

$$S_h(A)(X,Y) = \sum_{|\beta|<m} \frac{(\overline{Y}-\overline{X})^\beta}{\beta!} (\overline{\partial}^\beta \sigma_h^{wick}(A))(X) + \widetilde{R}_m(A; X, Y; h). \tag{8.8}$$

We shall restrict ourselves to the case where $A = Op_h^{weyl}(F)$ is a pseudo-differential operator.

Proposition 8.2. *Let A be an operator of the form $A = Op_h^{weyl}(F)$ where $F \in W^{\infty\infty}(\mathbb{R}^{2n})$. For all integer number $m \geq 1$, let $R_m(A; X, Y; h)$ and $\widetilde{R}_{mh}(A; X, Y; h)$ be the functions defined in (8.7) and (8.8). Then, there exists a function G_m in $L^1(\mathbb{R}^{2n})$ such that, for all h in $(0,1]$*

$$e^{-\frac{1}{4h}|X-Y|^2} |R_m(A; X, Y; h)| \ \leq \ G_m\left(\frac{X-Y}{\sqrt{h}}\right) \sum_{\alpha \in E_{mn}} h^{|\alpha|/2} \|\partial^\alpha F\|_{L^\infty(\mathbb{R}^{2n})}, \tag{8.9}$$

where E_{mn} is defined in (8.4). An analogous estimate remains valid for the function $\widetilde{R}_m(A; X, Y; h)$ defined in (8.8).

Proof. Proposition 4.4 gives an expression of the Wick symbol of $A_h = Op_h^{weyl}(F)$

$$\sigma_h^{wick}(A_h)(X) = (\pi h)^{-n} \int_{\mathbb{R}^{2n}} e^{-\frac{|X-Z|^2}{h}} F(Z) dZ$$

Since $S_h(A_h)(X,Y)$ is a function holomorphic in X, anti-holomorphic in Y and equaling to $\sigma_h^{wick}(A_h)$ on the diagonal, we necessarily have

$$S_h(A_h)(X,Y) = (\pi h)^{-n} \int_{\mathbb{R}^{2n}} e^{-\frac{1}{h}(Z-X).(\overline{Z}-\overline{Y})} F(Z) dZ.$$

In order to derive the Taylor expansion, we set for all $\theta \in [0,1]$

$$F_h(\theta, X, Y) = (\pi h)^{-n} \int_{\mathbb{R}^{2n}} F(Z) e^{\frac{1}{h}\varphi(\theta, X, Y, Z)} dZ,$$

$$\varphi(\theta, X, Y, Z) = -\Big(Z - Y - \theta(X-Y)\Big).(\overline{Z}-\overline{Y}) dZ.$$

Thus, we have $F_h(1, X, Y) = S_h(A_h)(X,Y)$ and $F_h(0, X, Y) = S_h(A_h)(Y,Y)$. The Taylor expansion is then written as

$$S_h(A_h)(X,Y) = \sum_{k<m} \frac{1}{k!} \partial_\theta^k F_h(0, X, Y) + R_m(A_h; X, Y; h),$$

$$R_m(A_h; X, Y; h) = \int_0^1 \frac{(1-\theta)^{m-1}}{(m-1)!} \partial_\theta^m F_h(\theta, X, Y)\ d\theta.$$

Differentiating the above equality through the integral and integrating by parts, we obtain:

$$\partial_\theta^k F_h(\theta, X, Y) = (\pi h)^{-n} \int_{\mathbb{R}^{2n}} e^{\frac{1}{h}\varphi(\theta,X,Y,Z)}\ \Big[(X-Y).\partial_Z\Big]^k F(Z)\ dZ.$$

Consequently,

$$\frac{1}{k!}\partial_\theta^k F_h(\theta, X, Y) = \sum_{|\alpha|=k} \frac{(X-Y)^\alpha}{\alpha!}(\pi h)^{-n} \int_{\mathbb{R}^{2n}} e^{\frac{1}{h}\varphi(\theta,X,Y,Z)}\ \Big(\partial^\alpha F\Big)(Z)\ dZ.$$

In particular, for $\theta = 0$,

$$(\pi h)^{-n} \int_{\mathbb{R}^{2n}} e^{\frac{1}{h}\varphi(0,X,Y,Z)}\ \partial_Z^\alpha F(Z)\ dZ = (\pi h)^{-n} \int_{\mathbb{R}^{2n}} e^{\frac{1}{h}|Y-Z|^2}\ \Big(\partial^\alpha F\Big)(Z)\ dZ$$

$$... = \Big(e^{\frac{h}{4}\Delta}\partial^\alpha F\Big)(Y) = \Big(\partial^\alpha \sigma_h^{wick}(A)\Big)(Y).$$

The Taylor remaining term is given by:

$$R_m(A_h; X, Y; h) = m \sum_{|\alpha|=m} \frac{(X-Y)^\alpha}{\alpha!}(\pi h)^{-n} \int_{[0,1]\times\mathbb{R}^{2n}} (1-\theta)^{m-1} e^{\frac{1}{h}\varphi(\theta,X,Y,Z)}\ \partial^\alpha F(Z)\ d\theta dZ.$$

Consequently,

$$\Big|R_m(A_h; X, Y; h)\Big|\ \leq\ m|X-Y|^m \left[\sum_{|\alpha|=m} \|\partial^\alpha F\|_{L^\infty}\right]\ (\pi h)^{-n} \int_{[0,1]\times\mathbb{R}^{2n}} (1-\theta)^{m-1} e^{\frac{1}{h}\mathrm{Re}\varphi(\theta,X,Y,Z)}\ d\theta dZ.$$

We see that:

$$\mathrm{Re}\varphi(\theta, X, Y, Z) = -\left|Z - Y - \frac{\theta}{2}(X-Y)\right|^2 + \frac{\theta^2}{4}|X-Y|^2.$$

If $m \geq n+1$ and $C > 0$ the following function

$$G_m(X) = C\ |X|^m \int_0^1 (1-\theta)^{m-1}\ e^{\frac{\theta^2-1}{4}|X|^2} d\theta$$

is in $L^1(\mathbb{R}^{2n})$. We can find $C > 0$ such that (8.9) is satisfied. When $m \leq n$ we have

$$R_m(A_h; X, Y; h) = R_{n+1}(A_h; X, Y; h) + \sum_{m \leq |\alpha| \leq n} \frac{(X-Y)^\alpha}{\alpha!}\Big(\partial_X^\alpha \sigma_h^{wick}(A)\Big)(Y).$$

When $m \leq n$ we can then find $C > 0$ such that the inequality (8.9) is verified when setting

$$G_m(X) = G_{n+1}(X) + C\ e^{-\frac{1}{4}|X|^2}\ \sum_{k=m}^{n} |X|^k$$

This function G_m is also in $L^1(\mathbb{R}^{2n})$. In both of the two cases we have the estimation (8.9). The estimation concerning $\widetilde{R}_m(A_h; X, Y; h)$ is similarly proved.

$\square$

End of the proof of theorem 8.1. Using (8.5) and using the asymptotic expansion in the first variable (here Y) of the function $S_h(A_h)(Y,X)$ given in the proposition 8.2 when $A_h = Op_h^{weyl}(F)$, we obtain:

$$\sigma_h^{wick}(A \circ B)(X) = \sum_{|\alpha|<m} \frac{a_\alpha(X,h)}{\alpha!} \partial^\alpha \sigma_h^{wick}(A)(X) + R_m(A,B;X;h)$$

where

$$a_\alpha(X,h) = (2\pi h)^{-n} \int_{\mathbb{R}^{2n}} \mathcal{B}_h(X,Y,Y,X)\ S_h(B)(X,Y)(Y-X)^\alpha dY$$

$$R_m(A,B;X;h) = (2\pi h)^{-n} \int_{\mathbb{R}^{2n}} \mathcal{B}_h(X,Y,Y,X)\ S_h(B)(X,Y) R_m(A;X,Y;h)\ dY.$$

From (4.9) we have:

$$\mathcal{B}_h(X,Y,Y,X) = \mathcal{B}_h(X,X,Y,X) = e^{-\frac{1}{2h}(X-Y)(\overline{X}-\overline{Y})}.$$

Therefore we obtain that

$$a_\alpha(X,h) = (2h)^{|\alpha|}(2\pi h)^{-n} \int_{\mathbb{R}^{2n}} S_h(B)(X,Y) \overline{\partial}_X^\alpha \mathcal{B}_h(X,Y,Y,X)\ dY$$

$$= (2h)^{|\alpha|}(2\pi h)^{-n} \overline{\partial}_X^\alpha \int_{\mathbb{R}^{2n}} \mathcal{B}_h(X,X,Y,X) S_h(B)(X,Y)\ dY$$

$$= (2h)^{|\alpha|} \overline{\partial}^\alpha \sigma_h^{wick}(B)(X).$$

We have used the fact that $\overline{\partial}_X S_h(B)(X,Y) = 0$ and the fact that the bi-symbol $S_h(B)$ verifies the property (8.6). Besides, from the bound of $R_m(A;X,Y;h)$ given by proposition 8.2,

$$|R_m(A,B;X;h)| \leq C_m(F,h)\ \ (2\pi h)^{-n} \int_{\mathbb{R}^{2n}} e^{-\frac{1}{4h}|X-Y|^2}\ |S_h(B)(X,Y)| G_m\left(\frac{X-Y}{\sqrt{h}}\right) dY,$$

$$C_m(F,h) = \sum_{\alpha \in E_{mn}} h^{|\alpha|/2} \|\partial^\alpha F\|_{L^\infty},$$

where G_m is a function in $L^1(\mathbb{R}^{2n})$. Consequently,

$$(2\pi h)^{-n} \int_{\mathbb{R}^{2n}} \Big| R_m(A,B;X;h) \Big|\ dX \leq ...$$

$$... \leq C_m(F,h)\ (2\pi h)^{-2n} \int_{\mathbb{R}^{4n}} e^{-\frac{1}{4h}|X-Y|^2}\ |S_h(B)(X,Y)| G_m\left(\frac{X-Y}{\sqrt{h}}\right) dX dY.$$

From proposition 4.3, the point concerning $A \circ B$ is proved and the one concerning $B \circ A$ is similarly derived. □

9. The equation satisfied by the Wick symbol of a solution to (TDHF).

If one only supposes that $\rho_h(t)$ is a classical solution to (TDHF) without assuming any additional hypothesis, then the Weyl symbol of $\rho_h(t)$ is a continuous function on $\mathbb{R}^{2n}$ with derivatives understood in the sense of distributions. However, from proposition 4.2 it is noted that its Wick symbol is in $W^{\infty 1}(\mathbb{R}^{2n})$ and therefore it is C^∞. We shall prove in this section that the Wick symbol satisfies a differential equation, with an asymptotic expansion in powers of h, the first term of the equation being the Vlasov equation, and the error term being as small as wanted, in terms of power of h, and of $L^1(\mathbb{R}^{2n})$. For the introduction ofsuch an equation, see [DLERS].

Proposition 9.1. *a) Let $\rho_h(t)$ be a classical solution to (TDHF). For all $t \in \mathbb{R}$ set:*

$$\varphi_h(X,t) = (2\pi h)^{-n}\ \sigma_h^{weyl}(\rho_h(t)) \tag{9.1}$$

$$u_h(X,t) = (2\pi h)^{-n}\ \sigma_h^{wick}(\rho_h(t)) \tag{9.2}$$

Then,

a) We have, in sense of distributions on $\mathbb{R}^{2n} \times \mathbb{R}$,

$$\frac{\partial \varphi_h}{\partial t} + 2\sum_{j=1}^{n} \xi_j \frac{\partial \varphi_h}{\partial x_j} = \frac{1}{ih}(2\pi h)^{-n} \sigma_h^{weyl}\Big([V_q(\rho_h(t)), \rho_h(t)]\Big). \tag{9.3}$$

b) We have:

$$\frac{\partial u_h}{\partial t} + 2\sum_{j=1}^{n} \xi_j \frac{\partial u_h}{\partial x_j} + h\sum_{j=1}^{n} \frac{\partial^2 u_h}{\partial x_j \partial \xi_j} = \frac{1}{ih}(2\pi h)^{-n} \sigma_h^{wick}\Big([V_q(\rho_h(t)), \rho_h(t)]\Big). \tag{9.4}$$

We observe that when the potentials are turned off ($V = W = 0$) then the Weyl symbol of $\rho_h(t)$ is the only one that exactly verifies Vlasov equation (but in the sense of distributions).

Proof. Point a) Let $\rho_h(t)$ be a classical solution of (TDHF). Let $u_h(.,t)$ be the function defined in (9.2). Let ψ be a C^∞ function with compact support in $\mathbb{R}^{2n} \times \mathbb{R}$. For all $t \in \mathbb{R}$, set $A_h(t) = Op_h^{weyl}(\psi(.,t))$. The mapping A_h is C^1 from $\mathbb{R}$ into $\mathcal{L}^1(\mathcal{H})$ and it is continuous from $\mathbb{R}$ into $\mathcal{D}$. We shall represent the integral

$$I_h = (2\pi h)^{-n} \int_{\mathbb{R}^{2n}\times\mathbb{R}} \varphi_h(x,\xi,t) \left[\frac{\partial \psi}{\partial t} + 2\sum_{j=1}^{n} \xi_j \frac{\partial \psi}{\partial x_j}(x,\xi,t) \right] dx d\xi dt.$$

We know that:

$$\sigma_h^{weyl}(h[\Delta, A_h(t)])(x,\xi) = 2i \sum_{j=1}^{n} \xi_j \frac{\partial \psi}{\partial x_j}(x,\xi,t).$$

Consequently, we have from (3.2),

$$I_h = \int_{\mathbb{R}} Tr\Big(\rho_h(t) \circ \big(A_h'(t) - ih[\Delta, A_h(t)]\big)\Big) dt.$$

Since the operators $\rho_h(t)$ and $A_h(t)$ are in $\mathcal{D}$, we have:

$$Tr\big(\rho_h(t)[\Delta, A_h(t)]\big) = -Tr\big([\Delta, \rho_h(t)] A_h(t)\big).$$

Consequently,

$$\begin{aligned} -I_h &= \int_{\mathbb{R}} Tr\Big(\big(\rho_h'(t) - ih[\Delta, \rho_h(t)]\big) \circ A_h(t)\Big) dt \\ &= \frac{1}{ih} \int_{\mathbb{R}} Tr\Big([V_q(\rho_h(t)), \rho_h(t)] \circ A_h(t)\Big) dt. \end{aligned}$$

Using (3.2) again,

$$-I_h = \frac{1}{ih}(2\pi h)^{-n} \int_{\mathbb{R}^{2n}\times\mathbb{R}} \sigma_h^{weyl}\Big([V_q(\rho_h(t)), \rho_h(t)]\Big) \varphi(x,\xi,t) dx d\xi dt.$$

Point b) Let $\rho_h(t)$ be a classical solution to (TDHF). Let $u_h(.,t)$ and $\varphi_h(.,t)$ be the functions defined in (9.1) and (9.2). We know (see proposition 4.4), that $u_h(.,t) = e^{\frac{h}{4}\Delta}\varphi_h(.,t)$. Applying the operator $e^{\frac{h}{4}\Delta}$ to the two hand-sides of (9.3) we obtain (9.4). □

Combining theorems 9.1 together with 8.1 and lemma 7.2 together with proposition 4.4 we directly obtain an equation satisfied by the Wick symbol of a solution to (TDHF) without any supplementary hypothesis and with an arbitrary high order of accuracy. However, without supplementary hypothesis, this equation does not allow to obtain an asymptotic expansion of the Wick symbol.

Theorem 9.2. *Let V and W be two potentials in $W^{\infty\infty}(\mathbb{R}^n)$. Let $\rho_h(t)$ be a classical solution to (TDHF) such that $\rho_h(0) \geq 0$. Let $u_h(.,t)$ be the function defined in (2.3). For all functions f in $L^1(\mathbb{R}^{2n})$, set:*

$$\Phi_h(f)(x) = (e^{\frac{h}{4}\Delta}V)(x) + \int_{\mathbb{R}^{2n}} W(x-y)f(y,\eta)dyd\eta.$$

Then the function u_h verifies, for all integer numbers $m \geq 2$:

$$\frac{\partial u_h}{\partial t} + 2\sum_{j=1}^{n} \xi_j \frac{\partial u_h}{\partial x_j} + h\sum_{j=1}^{n} \frac{\partial^2 u_h}{\partial x_j \partial \xi_j} = ...$$

$$... = \frac{1}{ih} \sum_{1\leq|\alpha|<m} \frac{(2h)^\alpha}{\alpha!} \Big[\partial^\alpha \Phi_h(u_h(.,t))\, \overline{\partial}^\alpha u_h(.,t) \;-\; \partial^\alpha w_h(.,t)\, \overline{\partial}^\alpha \Phi_h(u_h(.,t))\Big] + R_m(.,t,h)$$

where the function $R_m(.,t,h)$ is in $L^1(\mathbb{R}^{2n})$ for all $t \in \mathbb{R}$. For all $T > 0$, there exists $C_m(T) > 0$ such that:

$$(2\pi h)^{-n} \int_{\mathbb{R}^{2n}} \Big| R_m(X;h) \Big|\, dX \leq C_m(T) h^{\frac{m}{2}-1}.$$

10. The analogue of Ehrenfest's time.

The below result shows that the limit in corollary 2.2 cannot be uniform on $\mathbb{R}$, even without potentials V and W entirely vanishing, since exchanging there the two limits is false. In other words, according to the terminology of [BR], [dBR], the analogue of the Ehrenfest time for collary 2.2 is finite.

Theorem 10.1. *Let $h > 0$ be fixed. Let $\rho_h(t)$ be a classical solution to the (TDHF) equation corresponding to $V = W = 0$. We suppose that $\rho_h(0) \geq 0$ and assume that the trace of $\rho_h(0)$ equals 1. Let $u_h(.,t)$ and $v_h(.,t)$ be the functions defined in section 2. Then we have:*

$$\lim_{t\to\pm\infty} \|u_h(.,t) - v_h(.,t)\|_{L^1(\mathbb{R}^{2n})} = 2. \tag{10.1}$$

We recall here that the two functions $u_h(.,t)$ and $v_h(.,t)$ are in the unit ball of $L^1(\mathbb{R}^{2n})$.

Proof. When $V = W = 0$ the function $u_h(.,0)$ verifies from the proposition 9.1,

$$\frac{\partial u_h}{\partial t} + 2\sum_{j=1}^{n} \xi_j \frac{\partial u_h}{\partial x_j} + h\sum_{j=1}^{n} \frac{\partial^2 u_h}{\partial x_j \partial \xi_j} = 0. \tag{10.2}$$

The function $v_h(.,t)$ is the solution to the Vlasov equation equaling to $u_h(.,0)$ for $t = 0$. Then, $v_h(x,\xi,t) = u_h(x - 2t\xi, \xi, 0)$ in the case of vanishing potentials. Set

$$U_h(x,t) = \int_{\mathbb{R}^n} u_h(x + 2t\xi, \xi, t)d\xi. \tag{10.3}$$

We have:

$$\|u_h(.,t) - v_h(.,t)\|_{L^1(\mathbb{R}^{2n})} = \int_{\mathbb{R}^{2n}} |u_h(x+2t\xi,\xi,t) - u_h(x+2t\xi,\xi,t)| dx d\xi \geq \int_{\mathbb{R}^n} |U_h(x,t) - U_h(x,0)| dx.$$

From (10.2) and (10.3),

$$\frac{\partial U_h}{\partial t}(x,t) = -h \int_{\mathbb{R}^n} \sum_{j=1}^n \frac{\partial^2 u_h}{\partial x_j \partial \xi_j}(x+2t\xi,\xi,t) d\xi = 2ht\Delta_x U_h(x,t).$$

Consequently,

$$U_h(.,t) = e^{ht^2\Delta_x} U_h(.,0).$$

It is standard that:

$$\lim_{\lambda\to+\infty} \|e^{\lambda\Delta_x}F - F\|_{L^1(\mathbb{R}^n)} = 2\|F\|_{L^1(\mathbb{R}^n)},$$

if a function $F \geq 0$ is in $L^1(\mathbb{R}^n)$. The proof of the theorem is therefore completed.

□

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